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Inelastic Scattering Data for Major Actinides

Roberto Capote Noy
IAEA
Vienna, Austria

January 2019

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

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ABSTRACT

Tight target uncertainties on the inelastic scattering data for major actinides were derived from advanced reactor sensitivity studies, in particular for U-238 nucleus. A Consultant Meeting on "Inelastic Scattering and Capture Cross-section Data of Major Actinides in the Fast Neutron Region" was held at IAEA Headquarters, Vienna, Austria in 2011 where the situation was reviewed (see INDC(NDS)-0597: https://www-nds.iaea.org/publications/). The current meeting is a follow-up to review the status of on-going developments in optical model and statistical nuclear reaction modelling. Further issues in inelastic scattering modelling were discussed. It was concluded that advances in modelling are substantial, an inter-comparison of model calculations for non-fissile targets was recommended (e.g. for tungsten).

January 2019

Contents

1. Introduction

Nuclear data for energy applications continue to be of considerable interest to the IAEA. Sensitivity analyses for new reactor designs and for Accelerator Driven Systems further show that target uncertainties for certain nuclear data have to be very tight. This certainly applies to capture and inelastic scattering cross sections of the major actinides: ^{232}Th, ^{233,235,238}U, ^{239}Pu, and ^{240}Pu. It is therefore mandatory to provide nuclear data to the required accuracies together with reliable uncertainties. A previous Consultant Meeting was held in 2011 (see INDC(NDS)-0597: https://www-nds.iaea.org/publications/); this meeting is a follow-up.

The status of evaluated data files for inelastic scattering is still not satisfactory. Relatively large differences in evaluated inelastic cross sections are observed, therefore efforts are needed to improve the data.

Nine consultants attended the meeting. R. Capote Noy (IAEA, Vienna, Austria) served as Scientific Secretary, Ian Thompson (Livermore National Laboratory, USA) was elected Chairman of the meeting and T. Kawano (Los Alamos National Laboratory, USA) agreed to act as rapporteur. The approved Agenda is attached (Appendix I), as well as a list of participants and their affiliations (Appendix II).

2. Summary of Presentations by Participants

2.1. T. Kawano

Los Alamos National Laboratory, Los Alamos NM, USA

Kawano reported the statistical compound nuclear reaction theory for a deformed system. When we calculate nuclear reaction cross section for a system where nuclear deformation is involved, a simple regime of the spherical optical model plus the Hauser-Feshbach theory has to be extended to the coupled-channels scheme. In this case, the particle penetration is expressed in terms of Satchler's transmission matrix, which is no longer diagonal. We have been dealing with the direct reaction channels in the statistical model in an approximated way; the single-channel transmission coefficient from the coupled-channels method is defined as the probability of formation of compound nucleus on the ground state. Although this has a great advantage to reduce computational burden, quantitative validation of this simplification and understanding limitation are still needed.

A correct method to include the direct channels in the compound nuclear reaction is to diagonalize the transmission matrix by unitary transformation, called Engelbrecht-Weidenmueller transformation. Kawano performed this transformation for a Monte Carlo generated cross section ensemble based on the Gaussian Orthogonal Ensemble, GOE, together with the direct channel expressed by the K-matrix background. He confirmed that the approximated method indeed underestimates the calculated inelastic scattering cross section, as reported by Capote et al. He also demonstrated that this underestimation disappears when many reaction channels open, and the width fluctuation correction becomes negligible.

He noted that an exact GOE calculation for the deformed nuclei could be impractical. However, it was shown that an approximation by Moldauer gives almost identical results to the exact solution, which is convincing to employ this transformation in the existing Hauser-Feshbach codes. As an example, the Engelbrecht-Weidenmueller transformation with Moldauer's prescription was applied to the neutron-induced reaction on U-238, in which the radiative capture and fission channels are included. As expected, the compound inelastic scattering cross sections are 10-15% higher than the standard Hauser-Feshbach calculations.

2.2. NEA Data Bank activities, O. Cabellos

OECD/NEA Data Bank, Issy-Les-Moulineaux, France

Several studies confirm that inelastic scattering of major actinides, in particular of ^{238}U, has a significant impact in many fields of reactor physics and may affect several key-parameters such as power map, absorber efficiency, kinetics parameters, Na void effect, Doppler…

The unique entry for inelastic scattering data of major actinides in the WPEC/High Priority Request List (HPRL) is dated from 2008. For this request, the ^{238}U (n,n') cross-section in the incident range from 65keV to 20 MeV is an important issue that emerges from different nuclear systems assessed in WPEC/SG26 ("*Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations*"). There is a high sensitivity for estimates of keff for the GFR ("*gas-cooled fast reactor*"), LFR ("*lead-cooled fast reactor*"), ABTR ("*advanced breeder test reactor*") and SFR("*sodium-cooled fast reactor*"). It concludes that an uncertainty of ±5% on ^{238}U(n,n') is required to reach the target uncertainties.

Recently, new studies support the need of this improvement. In **JEFDOC-1574**, ("*Uncertainty in PWR Calculations. Needs for nuclear data improvement*" by A. Santamarina) the ^{238}U(N,n') is identified as the main contributor to power map uncertainty between 3% to 5% at PWR centre. It is noted an increase of the uncertainty on the power map with the size of the core, from 5% (900MWe) to 10% (1450MWe). Regarding the impact on kinetic parameters, **JEFDOC-1476** *("βeff sensitivity-uncertainty analysis and its use for nuclear data evaluation and validation*" by I. Kodeli) highlighted the contribution in the β_{eff} uncertainty of ^{238}U(n,n'), between 2-3%.

In Fig. 1, a comparison between different evaluated libraries shows differences in the range of 1-5 MeV of around 8%. In **JEFDOC-1674** ("*EXCALIBUR An Integral Experiment for ^{238}U(n,n'). Validation at CALIBAN*" by P. Leconte) several sensitive integral experiments were analysed to suggest a probable overestimation of ^{238}U(n,n') by ~10% in JEFF-3.1.1.

In addition, there is no consensus on the ^{238}U(n,n') covariance data to be adopted in the 2-5 MeV range of maximum sensitivity for reactor applications (see Fig.2).

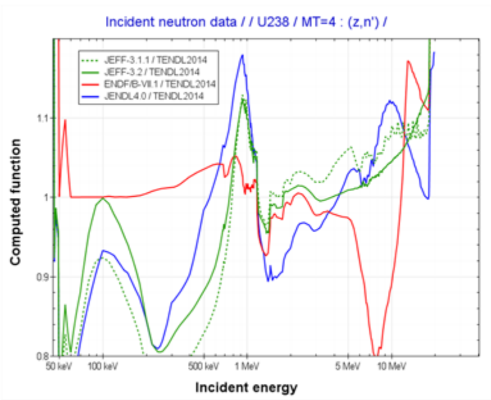


Fig. 1. Ratio between different evaluations

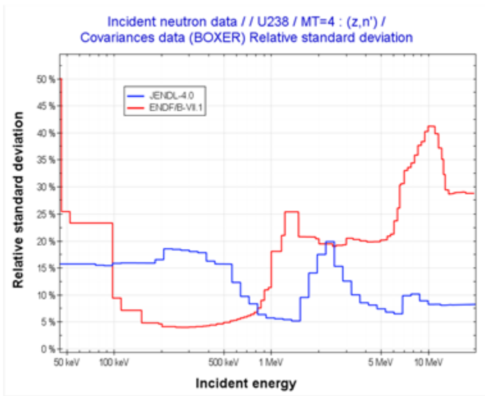


Fig. 2. Comparison of standard deviation

Evaluation activities in other minor actinides (^{240}Pu, ^{237}Np,..) have been performed in the last years in the framework of the JEFF and WPEC projects. Recently, sensitivity an uncertainty analysis for the prediction of ^{241}Am critical mass indicated additional needs on ^{241}Am inelastic cross-section evaluations (**WPEC/SG39-2015**, "*keff uncertainties for a simple case of ^{241}Am using different codes and evaluated files*" by I. Kodeli). Differences in k_{eff} between ENDF/B-VII.0 and JENDL-4.0 are around 3.5%Δk/k. However, the sensitivities calculated using ENDF/B-VII.0 and JENDL-4.0 are in fair agreement. Large differences in k_{eff} uncertainties were observed between uncertainties based on different covariance matrix evaluations: COMMARA-2: ~3%, SCALE-6.0: ~ 7.5% and JENDL-4.0: ~ 5.5%. The most important contributor in JENDL-4.0m and ENDF/B-VII.0 is PFNS, 5.1% and 5.8%, respectively. The top contributor in SCALE-6.0 is $^{241}Am(n,n')$.

In this context, the OECD/NEA Data Bank's nuclear data services and the OECD/Nuclear Science programme through the Working Party on International Evaluation Co-operation (WPEC) have launched several activities focused on evaluated nuclear data activities. Some of these activities are of particular interest to this project:

- Enhancing the Joint Evaluated Fission and Fusion (JEFF) project. **JEFF-3.3** will be released in 2018 with improvements in nuclear theory and evaluation, including more relevant and recent experiments.
- Organizing bi-annual **JEFF Nuclear Data Weeks** joint with other projects (e.g. GEDEPEON, NEEDS, CHANDA), and contributing to the organisation of external workshops (e.g. WONDER 2015)
- Checking, processing, verification, validation, benchmarking and diagnosis of evaluated nuclear data will be performed with the implementation of the new **Evaluated Nuclear Data Evaluation Cycle** (NDEC) platform.
- For integral benchmarking, the selection of pertinent criticality benchmarks (for some nuclide/reaction specific, above a given sensitivity threshold to keff) from ICSBEP/DICE and diagnosis analysis through **Nuclear Data and Sensitivity Testing Tool** (NDaST). NDaST will provide rapid predictions of the integral responses (e.g Δkeff) to changes in nuclear data. These changes could be direct both perturbations of nuclear data and nuclear covariance data uncertainties.
- **WPEC/CIELO** ("*Collaborative International Evaluated Library Organisation Pilot Project*") where inelastic scattering discrepancies between evaluations for actinides are a very important issue. CIELO project will review various theoretical approaches and optical model options. Regarding experiments, RPI's measurements using a semi-integral approach have had a large impact on validating and improving inelastic and elastic scattering on ^{238}U. From benchmarking, the main objective is to understand the implications in k_{eff} and reaction rates from integral data testing on changes in (n,n').
- **WPEC/SG39** ("*Methods and approaches to provide feedback from nuclear and covariance data adjustment for improvement of nuclear data files*") is assessing current covariance nuclear data in evaluated libraries, and developing adjustment methodologies to avoid compensating effects. The WPEC/SG39 has recently revised the status of the covariance data of JENDL-4.0 and ENDF/B-VII.1, and it has revealed large differences for the standard deviation values and the correlation matrix.
- **WPEC-SGC** ("*Expert Group on the High Priority Request List for Nuclear Data*") is working on new request for inelastic scattering in ^{239}Pu, ^{235}U and other actinides.

2.3. Optical potentials comparisons, P. Romain and B. Morillon

CEA/DAM/DIF, Arpajon Cedex, France

As discussed in 2011 at the IAEA (http://int-nds.iaea.org/publications/indc/indc-nds-0597.pdf) Technical Meeting on Inelastic Scattering Cross-Section Data of Major Actinides in the Fast Neutron Region, we know that the optical model plays a dominant role in the description of the inelastic cross section.

Hence in this present study devoted to ^{239}Pu and ^{235}U, we compare two different dispersive optical potentials in the coupled channel framework (DCCOMP), as required for actinides. We do not only restrict ourselves to the DCCOMP results, but since interested by inelastic scattering cross sections, we investigate a step further by testing the deduced transmission coefficients in statistical calculations running the TALYS code with the same TALYS-input statistical parameters for a given nucleus. Thus, differences are only due to DCCOMP calculations.
Our BRC-DCCOMP calculations for ^{235}U use a 7-levels coupling scheme: 5 ground states rotational band (7/2-, 9/2-,11/2-,13/2-,15/2-) coupled with the (7/2+,9/2+) states that we treat (poor assumption) as octupolar vibrational states. In the same way for ^{239}Pu, we use a 9-levels coupling scheme: 5 ground states rotational band (1/2+, 3/2+,5/2+,7/2+,9/2+) coupled with the 4 (1/2-,3/2-,5/2-,7/2-) states, again treated (poor assumption) as octupolar vibrational states. R. Capote OPTMAN-DCCOMP calculations use more complex and larger coupling schemes (19 levels (4 bands) for ^{239}Pu and 21 levels (4 bands) for ^{235}U) see [1].

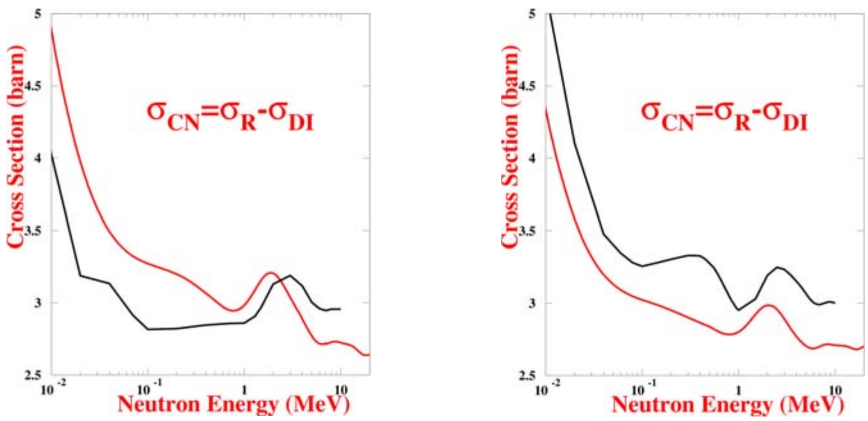


Fig. 1 : Compound Nucleus formation cross sections for ^{235}U (left) and ^{239}Pu (right) calculated with our BRC-CCDOMP (red) and OPTMAN-CCDOMP (black) (Ref. [1]).

As shown on Fig. 1, Compound Nucleus formation cross sections look rather different from one CCDOMP to another. As example the maxima positions (around 2 MeV) are energy shifted. This could have an effect when calculating fission cross sections, see Fig. 2. Indeed, the energy position of the bumps around 2 MeV in the BRC compound nucleus formation cross sections seems more appropriate to reproduce the bumps (around 2 MeV) in the fission cross sections compared to the OPTMAN one. Another big difference is the bump around 400 keV in the OPTMAN-CCDOMP Compound Nucleus formation cross section of ^{239}Pu compared to BRC-CCDOMP calculations, see Fig 1.

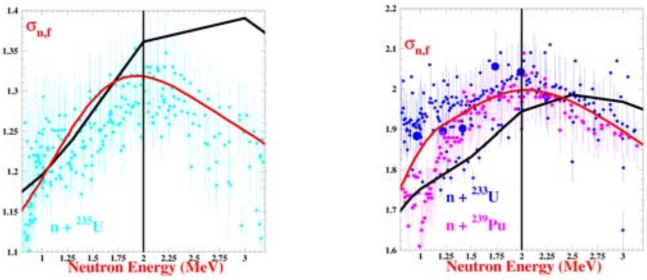


Fig. 2 : Induced neutron fission cross sections around 2 MeV, where the experimental data present a bump. BRC-TALYS (red curves) calculations compared to OPTMAN-TALYS (balck curves) calculations.

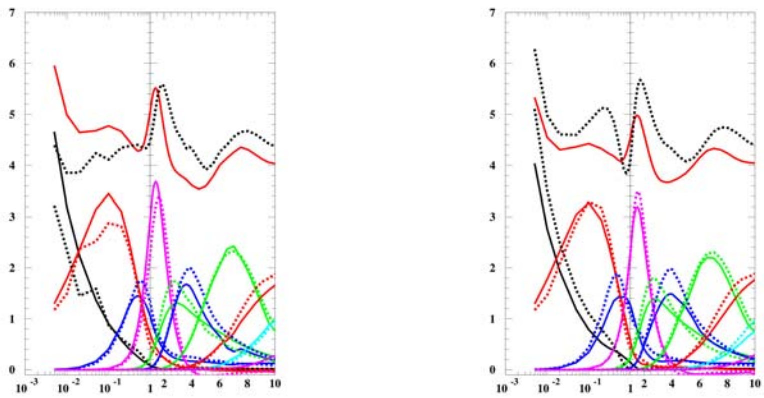
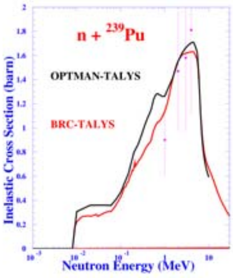


Fig. 3: Energy derivative of EσCN (red continuous and black dashed curves at the top) and energy derivative of each partial wave component (2l+1)Tl (all bottom curves, from left to right l=0:black, l=1:red, l=2:blue, l=3:magenta, l=4:green, l=5:blue, l=6:green, l=7:red, l=8:cyan, l=9:magenta). All continuous curves correspond to BRC-CCDOMP calculations and all dashed curves to the OPTMAN-CCDOMP calculations.

An interesting study is the analysis of the energy derivative of the compound nucleus formation cross section multiplied by energy, or more precisely the energy derivative of each term of the sum, i.e. of each component defined by $(2l+1)T_l$, this defines a kind of centrifugal barriers distribution. Thus from Figs 1 and 3, it appears that the bump around 2 MeV in all Compound Nucleus formation cross sections could be due to a large absorption of l=3 waves (large magenta peaks around 2 MeV on figure 3). On the same way the bump around 400 keV in the OPTMAN-CCDOMP Compound Nucleus formation cross section of ^{239}Pu could be due to a larger absorption of (l=2) d-waves and (l=0) s-waves too, compared to BRC-CCDOMP (see black and blue dashed curves at the right bottom part of figure 3). Even if this bump seems induce larger inelastic and fission cross sections (Fig. 4) in this energy range, nothing allows to conclude definitively that that is wrong.



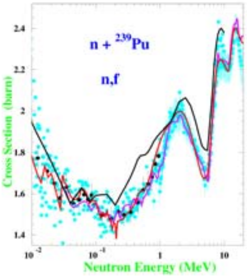


Fig. 4: BRC-TALYS (red curves) and OPTMAN-TALYS (black curves) inelastic (left) and fission (right) calculated cross sections, both with the same TALYS-input statistical parameters, thus meaning that differences are only due to CCDOMP calculations.

[1] J.M. Quesada, R. Capote, E.Sh. Soukhovitskii, S. Chiba, Nucl. Data Sheets **118** (2014) pp. 270-272

2.4. Uncertainties in Actinide Optical Potentials, I. Thompson

Lawrence Livermore National Laboratory, Livermore CA, USA

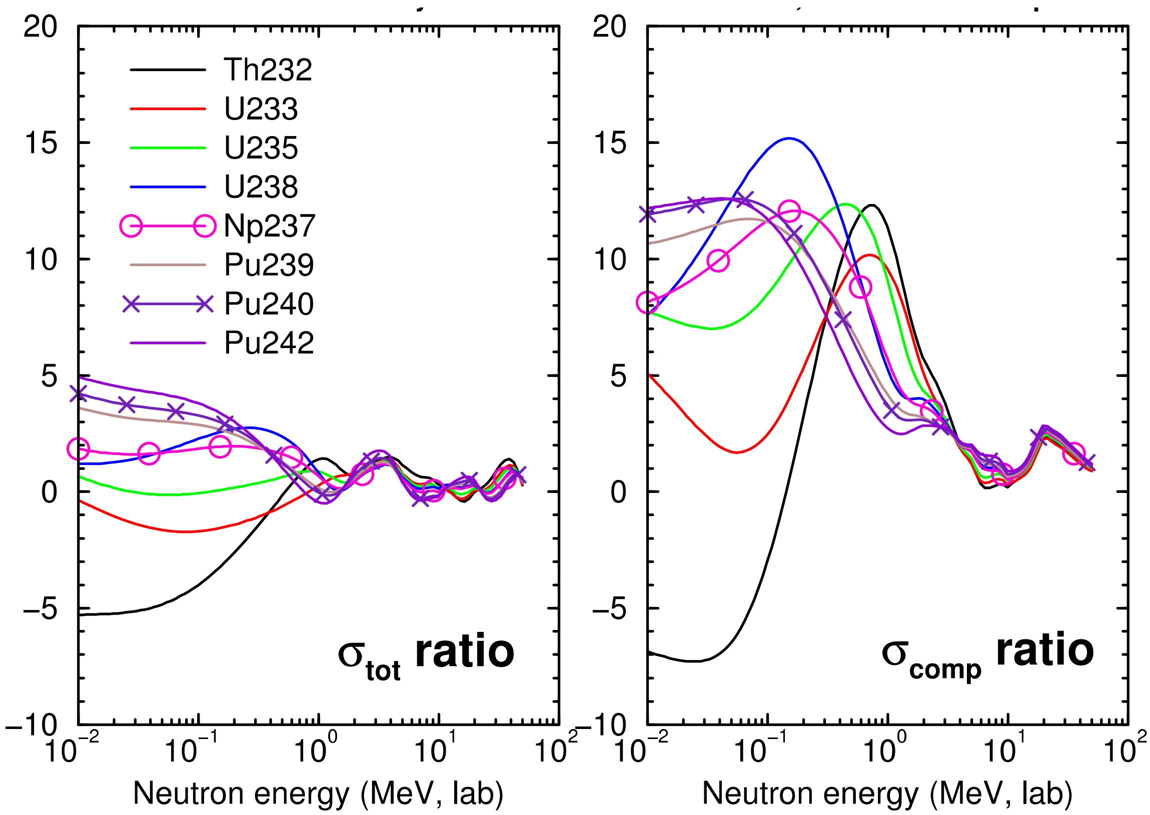
The inelastic (n,n′) reactions on actinide nuclei cannot easily be measured, especially those which populate states of low excitation energies. Model calculations are therefore need to interpolate between (and extrapolate from) the data for those discrete and continuum states that can be measured. Such models are critically dependent on several ingredients: the choice of neutron optical potentials, the collective deformations of these deformed actinides, and the level densities. I here focus on uncertainties arising from the optical potentials, especially when different optical potentials may be fitted almost as well to the same data, yet produce different predictions for what must be inferred indirectly.

At the NEMEA-7 conference in 2013, I reported (Thompson et al, 2014) on a generalization of Dietrich's FLAP2.2 regional optical potential (Escher et al, 2010). This revision is necessary because Dietrich et al (2012) showed that the convergence of coupled-channel calculations is much slower than was previously believed. Many more states needed for convergence than, for example, the ground state plus 2 levels used for FLAP 2.2 and in default TALYS calculation. That fact requires us to re-examine the fit to neutron data for scattering on actinides, now using fully converged coupled-channels calculations with at least 6 or 7 levels for even-even nuclei, and about twice that number for odd nuclei. In 2013 I therefore reported on a generalization we call FLAP 3.0, which kept the format of isospin dependence in a Lane-consistent formalism, and describing energy dependence by a linear dependence of Saxon-Woods parameters in 6 ranges up to 50 MeV. The specified energy dependence improves the consistency with the dispersion relations that link the real and imaginary components. Our potential was initially based on the Koning and Delaroche (2003) global nucleon-nucleus potential, but added some minor parameter modifications at low energies to improve the fit to the σ_{TOT} data for ^{238}U. That Koning-Delaroche potential has imaginary parts that go to zero quadratically at the Fermi surface E_F of each nuclide.

As well as the optical parameters and the energy of the Fermi surface, we need deformations: principally β_2 and β_4. For these, we started with the results of coupled-channel fits of charged-particle scattering ^{238}U(p,p′) at higher energies. Fits to that data gives average values of $\beta_2 = 0.2323$ and $\beta_4 = 0.045$. To extend to other targets, those numbers where used to rescale the deformations extracted from the B(E2) decay measurements published by Raman. The β_4 were kept the same as for ^{238}U.

The resulting fits for the σ_{TOT} data for ^{232}Th, ^{233,225,238}U and ^{239,240}Pu were good as a preliminary fit. However, the fit got significantly worse when, instead of the ^{238}U Fermi energy, the better nucleus-specific Fermi energies were used according to $E_F = -(S_n(A,Z)+S_n(A+1,Z))/2$. The global fit could be recovered, however, if instead of using β_4 = 0.045 for all nuclei, we used instead the β_4 values fitted by Soukhovitskii (2004) to each nucleus separately for his potential. That is, I am using *his* β_4, but with the FLAP 3.0 geometry, and find again some good fits.

The result of this process is that we now have two 6-nucleus regional fits to actinide σ_{TOT} data: Soukhovitskii (2004) and also FLAP 3.1 as we call FLAP 3.0 with the new deformations. The β_4 deformations are shared, but all the other potential strengths and geometries are different, but we find that the fits are generally equivalent in accuracy. That is, however, accuracy for total cross sections, for the compound-nucleus cross sections are very different. The figure shows the percentage (%) deviations between the two evaluations, for (on the left) total and (on the right) compound-nucleus production cross sections. We see that the variations between the compound cross sections are general 5 to 10 times larger than between the total cross sections, especially for neutron energies below 2 MeV.



The large difference on the right shows the model dependence of the connection between the measured total cross sections and the predicted compound cross sections. These are the cross sections that are so important for inelastic and all other compound reaction channels. The large uncertainties in the compound cross sections can be reduced by using neutron strength functions S_0 and S_1, should the target be sufficiently stable that these can be measured. They can be reduced by more accurate total cross section measurements, but only in part because of the model dependencies shown above. Measurements of specific non-elastic channels will also help.

On the basis of existing measurements, we must conclude that there are still significant uncertainties in the compound nucleus cross sections in our region of interest below 2 MeV. Model uncertainties must contribute a large part to the overall error estimates. Deformations may well be obtainable from density-functional theories, including both k=2 and k=4 deformations, provided the theoretical multipole moments can be accurately translated to the β_k for the deformed rotor models used in coupled-channel calculations.

3. Recommendations

Theory

1. Demonstrate the effect of multiband coupling on the compound nucleus formation cross section.
2. Clarify the role of the deformation parameters and model assumptions of the collective model. How should these be determined from data and how do they relate to predictions/systematics?
3. Investigate if the QRPA results can be approximated to allow pragmatic calculations for actinides. Can they be extended to include 4qp, 6qp, … (and where should it stop)?
4. Hauser-Feshbach calculations should be modified to use the Engelbrecht-Weidenmueller transformation. The Moldauer formula should be used with the LANL parameterization of the degrees of freedom.
5. Establish the range of variation in compound formation cross section by fitting the data with different models.
6. Investigate if the dispersion relation helps to reduce the range of variation discussed in point 5.
7. Investigate which model assumptions are critical for the prediction of (n,n'g), (n,xng) and isomer data.
8. Establish the correct link between resonance parameters and the optical model parameters at low-energy.
9. Contribute to point 5 by an inter-comparison for W-186.
10. Benchmark data for tungsten may be used as a check.

Experiment

1. Data needed to confirm trend EW-transformation at energies between 45 and 1000 keV (U-238). The effect could be studied for a W-isotope.
2. Data RPI-style for U-235, Pu-239 (Th, W) are of interest to benchmark models. This type of measurement should be extended to cover low-energy emitted neutrons (0.1-1 MeV range). The motivation concerns systematic differences found for U-238, Therefore, U-238 also needs checking.
3. Other neutron scattering measurements should be encouraged.
4. Validation experiments should be encouraged, eg. EXCALIBUR. This type of measurement for W would be interesting.
5. Scattering on different thickness samples?
6. Update/add to HPRL entries.

Actions

It is recommended to organize OMP intercomparison for W isotopes, conclusions may be contributed to discussions within the RIPL project.

Appendix 1

CONSULTANCY MEETING ON INELASTIC SCATTERING DATA OF MAJOR ACTINIDES

VIENNA, 22- 23 JUNE 2015
VIC, ROOM M0E61
AGENDA

Monday, 22 June		
08:30 – 09:30	**Registration**	(IAEA Registration desk, Gate 1)
09:30 – 10:00	**Opening Session** Welcoming address and introduction Election of Chairman and Rapporteur Adoption of Agenda	R. Capote (Deputy SH, NDS)
10:00 – 12:45	**Presentations by participants**	
12:45 – 13:00	Administrative matters	
13:00 – 14:00	*Lunch Break*	
14:00 – 18:00	**Presentations by participants (cont'd)**	
	Coffee Break as needed	

Tuesday, 23 June		
09:00 – 13:00	**Presentations by participants (cont'd)**	
	Coffee Break as needed	
13:00 – 14:00	*Lunch Break*	
14:00 – 17:30	**Status of inelastic cross sections and data needs: recommendations**	
17:30	Closing of the meeting	
	Coffee Break as needed	

Appendix 2

Consultancy Meeting on Inelastic Scattering Data of Major Actinides

IAEA, Vienna, Austria
22 – 23 June 2015

List of participants

BELARUS
Efrem SOUKHOVITSKI
Nuclear Data Evaluation Lab
Joint Institute of Energy and Nuclear Research Academician A. K. Krasin, 99
220109 MINSK
Tel:+
E-mail: esukhov@sosny.bas-net.by

BELGIUM
Arjan PLOMPEN
SN3S Unit
IRMM-JRC-EC
Retieseweg 111
GEEL 2440
BELGIUM
Tel: +3214571381
E-mail: Arjan.Plompen@ec.europa.eu

FRANCE
Pascal ROMAIN
DEA DAM DIF
ARPAJON 91297
FRANCE
Tel: +
E-mail: 'Pascal.ROMAIN@CEA.FR'

Oscar CABELLOS
OECD Nuclear Energy Agency Databank
Le Seine Saint-Germain
12, boulevard des Iles
ISSY-LES-MOULINEAUX 19130
FRANCE
Tel: +
E-mail: cabellos@din.upm.es

FRANCE
Gilles NOGUERE
CEA/DEN Cadarache
ST. PAUL LEZ DURANCE 13108
FRANCE
Tel: + 33442252777
E-mail: gilles.noguere@cea.fr

JAPAN
Osamu IWAMOTO
Japan Atomic Energy Agency
Nuclear Data Center
TOKAI-MURA, NAKA-GUN
IBARAKI-KEN 319-1195
JAPAN
Tel:
E-mail: iwamoto.osamu@jaea.go.jp

ROMANIA
Mihaela SIN
Bucharest University
P.O. Box MG-11
BUCHAREST-MAGURELE 76900
ROMANIA
Tel:+40314574666
E-mail: mihaela.sin@gmail.com

UNITED STATES OF AMERICA
Ian THOMPSON
Lawrence Livermore National Laboratory (LLNL)
LIVERMORE, CA
Tel: +
E-mail: thompson97@llnl.gov

UNITED STATES OF AMERICA

Toshihiko KAWANO
T2, MS B2, Theoretical Div.
LOS ALAMOS NM 87545
UNITED STATES OF AMERICA
Tel: +
E-mail: Kawano@lanl.gov

IAEA

Roberto CAPOTE NOY
IAEA Nuclear Data Section
Vienna International Centre
PO Box 100
1400 Vienna
Tel: + 43-1-2600-21713
Fax:+ 43-1-26007
E-mail: Roberto.CapoteNoy@iaea.org

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://www-nds.iaea.org